LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU073119\
Data File : VU033519.D
Acq On : 31 Jul 2019 12:39
Operator : JC/SP
Sample : K4103-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DB9D6

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM073119WMA.M
Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.286	53	61	78	rBV	30812	74030	3.53%	0.585%
2	1.389	87	93	108	rVB	169882	179827	8.58%	1.421%
3	1.669	173	180	197	rVB	142685	177331	8.46%	1.401%
4	2.257	352	363	377	rVB	272286	408925	19.52%	3.230%
5	2.434	412	418	421	rBV4	930	1114	0.05%	0.009%
6	2.521	442	445	448	rBV	241	192	0.01%	0.002%
7	2.556	452	456	459	rBV2	191	193	0.01%	0.002%
8	2.624	473	477	485	rBV3	565	524	0.03%	0.004%
9	2.685	490	496	500	rBV3	548	608	0.03%	0.005%
10	2.723	505	508	515	rVB3	398	475	0.02%	0.004%
11	2.826	526	540	547	rBV4	1004	2304	0.11%	0.018%
12	2.968	577	584	594	rVB4	1523	2611	0.12%	0.021%
13	3.325	688	695	699	rVB2	174	212	0.01%	0.002%
14	3.366	704	708	711	rBV2	232	185	0.01%	0.001%
15	4.196	937	966	993	rBV2	568652	1643514	78.45%	12.984%
16	4.466	1047	1050	1054	rVB2	402	304	0.01%	0.002%
17	4.524	1063	1068	1072	rVB2	599	553	0.03%	0.004%
18	4.620	1081	1098	1120	rBV	195978	460174	21.97%	3.635%
19	4.768	1141	1144	1146	rBV2	408	318	0.02%	0.003%
20	4.807	1153	1156	1159	rVB3	545	296	0.01%	0.002%
21	4.849	1165	1169	1170	rBV2	668	411	0.02%	0.003%
22	4.964	1202	1205	1207	rBV2	477	219	0.01%	0.002%
23	5.032	1221	1226	1228	rBV2	242	218	0.01%	0.002%
24	5.315	1291	1314	1341	rBV2	394687	1153633	55.07%	9.114%
25	5.514	1373	1376	1379	rBV	371	214	0.01%	0.002%
26	5.640	1412	1415	1421	rBV4	412	436	0.02%	0.003%
27	5.723	1437	1441	1443	rBV4	494	367	0.02%	0.003%
28	5.746	1446	1448	1455	rVB	475	424	0.02%	0.003%
29	5.794	1460	1463	1468	rVB3	250	246	0.01%	0.002%
30	5.865	1468	1485	1508	rBV	361703	713797	34.07%	5.639%
31	6.164	1563	1578	1609	rBV	1095278	2094889	100.00%	16.550%
32	6.308	1609	1623	1646	rVB	262498	521702	24.90%	4.121%
33	6.501	1681	1683	1688	rVB3	590	469	0.02%	0.004%
34	6.524	1688	1690	1692	rBV	398	237	0.01%	0.002%

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Instrument : MSVOA_U
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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM073119WMA.M
Title : VOC Analysis

35	6.807	1774	1778	1781	rBV3	276	217	0.01%	0.002%
36	6.852	1785	1792	1795	rBV2	557	594	0.03%	0.005%
37	6.874	1795	1799	1801	rBV	320	242	0.01%	0.002%
38	6.907	1806	1809	1812	rVB	341	178	0.01%	0.001%
39	6.945	1819	1821	1826	rBV2	347	273	0.01%	0.002%
40	6.974	1827	1830	1835	rVB2	268	248	0.01%	0.002%
41	7.003	1835	1839	1842	rBV	268	262	0.01%	0.002%
42	7.096	1863	1868	1871	rBV2	200	188	0.01%	0.001%
43	7.144	1878	1883	1886	rBV3	273	240	0.01%	0.002%
44	7.209	1890	1903	1929	rBV	141664	258308	12.33%	2.041%
45	7.337	1940	1943	1949	rBV4	421	392	0.02%	0.003%
46	7.386	1953	1958	1961	rBV4	373	441	0.02%	0.003%
47	7.546	1995	2008	2037	rBV	528802	919297	43.88%	7.262%
48	7.759	2071	2074	2080	rVB3	547	466	0.02%	0.004%
49	7.833	2085	2097	2124	rBV	102963	180038	8.59%	1.422%
50	8.064	2164	2169	2173	rBV3	252	257	0.01%	0.002%
51	8.164	2187	2200	2212	rBV2	13527	25495	1.22%	0.201%
52	8.292	2230	2240	2276	rBV	340638	591714	28.25%	4.675%
53	8.498	2302	2304	2308	rVB2	377	220	0.01%	0.002%
54	8.550	2317	2320	2322	rVB3	363	189	0.01%	0.001%
55	8.717	2368	2372	2374	rBV3	257	176	0.01%	0.001%
56	8.820	2401	2404	2408	rBV3	314	308	0.01%	0.002%
57	8.910	2428	2432	2438	rVB2	255	247	0.01%	0.002%
58	9.006	2457	2462	2465	rBV2	204	203	0.01%	0.002%
59	9.070	2468	2482	2522	rBV	544302	899804	42.95%	7.108%
60	9.360	2567	2572	2573	rVV2	286	234	0.01%	0.002%
61	9.678	2669	2671	2676	rVB	279	197	0.01%	0.002%
62	9.720	2676	2684	2688	rBV3	343	413	0.02%	0.003%
63	9.749	2691	2693	2695	rVV2	392	209	0.01%	0.002%
64	9.765	2695	2698	2702	rVB2	210	183	0.01%	0.001%
65	9.839	2718	2721	2726	rBV2	230	189	0.01%	0.001%
66	9.865	2726	2729	2736	rVB	214	215	0.01%	0.002%
67	9.900	2736	2740	2744	rBV2	326	323	0.02%	0.003%
68	10.154	2817	2819	2822	rVB2	435	255	0.01%	0.002%
69	10.279	2855	2858	2863	rBV	266	187	0.01%	0.001%
70	10.331	2869	2874	2876	rBV2	362	300	0.01%	0.002%
71	10.414	2888	2900	2917	rBV	385018	618926	29.54%	4.889%

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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM073119WMA.M
Title : VOC Analysis

72	10.495	2923	2925	2930	rVB4	434	335	0.02%	0.003%
73	10.546	2936	2941	2944	rBV2	240	248	0.01%	0.002%
74	10.594	2945	2956	2971	rVB3	13212	21438	1.02%	0.169%
75	10.649	2971	2973	2977	rBV3	431	245	0.01%	0.002%
76	10.758	3003	3007	3011	rVB2	423	381	0.02%	0.003%
77	10.791	3011	3017	3019	rBV	314	351	0.02%	0.003%
78	10.913	3052	3055	3058	rBV2	247	239	0.01%	0.002%
79	11.115	3113	3118	3120	rBV2	346	283	0.01%	0.002%
80	11.215	3145	3149	3154	rVB3	313	262	0.01%	0.002%
81	11.276	3164	3168	3169	rBV	299	238	0.01%	0.002%
82	11.340	3186	3188	3191	rVB	386	210	0.01%	0.002%
83	11.369	3191	3197	3198	rBV2	268	244	0.01%	0.002%
84	11.408	3206	3209	3212	rVB3	806	628	0.03%	0.005%
85	11.466	3216	3227	3250	rBV	525366	835717	39.89%	6.602%
86	11.758	3315	3318	3320	rBV2	312	196	0.01%	0.002%
87	11.842	3329	3344	3366	rBV	527538	849600	40.56%	6.712%
88	12.054	3405	3410	3411	rBV3	307	258	0.01%	0.002%
89	12.196	3451	3454	3459	rVB4	587	475	0.02%	0.004%
90	12.218	3459	3461	3463	rBV2	314	193	0.01%	0.002%
91	12.646	3591	3594	3599	rVB4	393	306	0.01%	0.002%
92	12.836	3648	3653	3657	rBV2	378	408	0.02%	0.003%
93	12.884	3661	3668	3677	rVB4	737	1347	0.06%	0.011%
94	12.942	3684	3686	3692	rVB3	309	234	0.01%	0.002%
95	13.022	3709	3711	3714	rVB2	385	214	0.01%	0.002%
96	13.414	3831	3833	3839	rBV2	287	211	0.01%	0.002%
97	13.742	3932	3935	3937	rBV	439	338	0.02%	0.003%
98	13.845	3964	3967	3970	rBV3	499	427	0.02%	0.003%
99	13.906	3983	3986	3991	rBV4	402	422	0.02%	0.003%
100	14.196	4073	4076	4078	rBV	389	250	0.01%	0.002%

Sum of corrected areas: 12658278

LSC Report - Integrated Chromatogram

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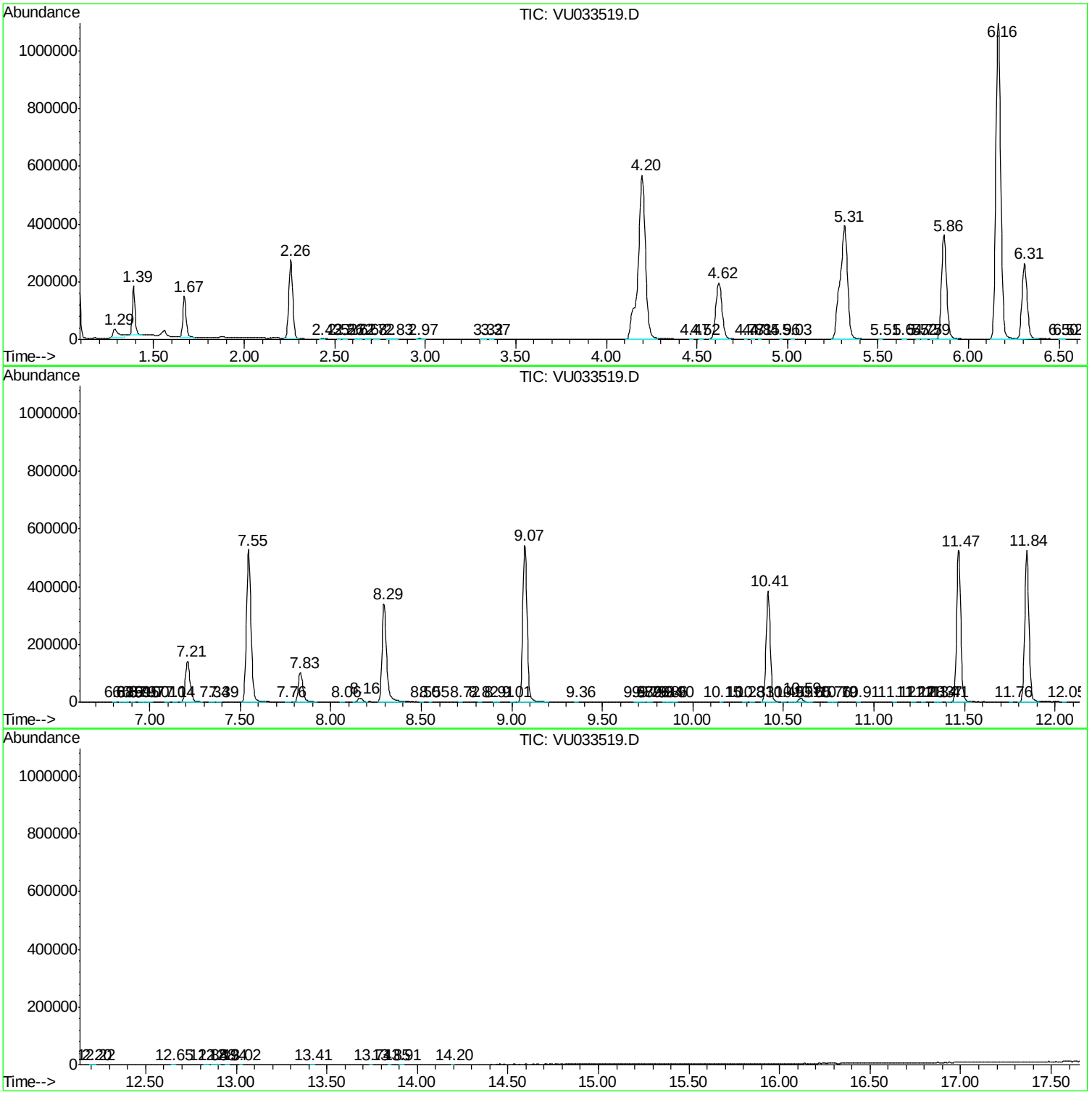
Instrument : MSVOA_U
ClientSampleId : DB9D6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM073119WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU073119\
Data File : VU033519.D
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Operator : JC/SP
Sample : K4103-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DB9D6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM073119WMA.M
Quant Title : VOC Analysis

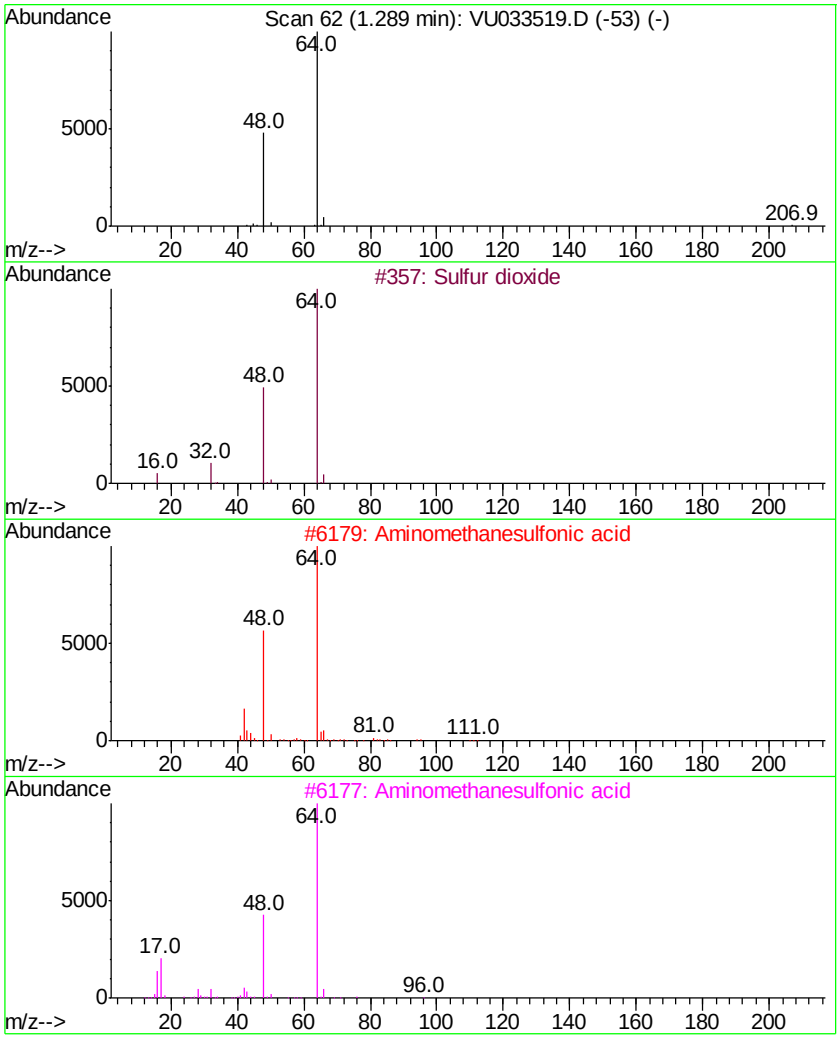
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

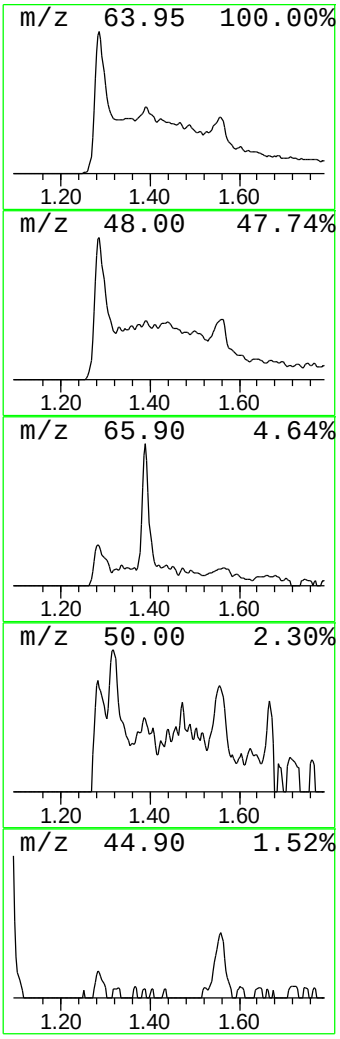
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.29	5.19 ug/L	74030	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Sulfur dioxide	64	O2S	007446-09-5	3





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.29	5.2	ug/L	74030	1	5.86	713797	50.0